Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 07:19:28 ON 07 MAY 2007

=> file reg
COST IN U.S. DOLLARS

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 0.42 0.42

FILE 'REGISTRY' ENTERED AT 07:20:51 ON 07 MAY 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 MAY 2007 HIGHEST RN 934336-20-6 DICTIONARY FILE UPDATES: 6 MAY 2007 HIGHEST RN 934336-20-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

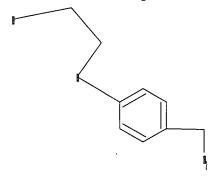
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

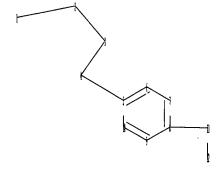
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

Uploading C:\Documents and Settings\mgraffeo\My Documents\Critical Data\10814058\cmp 2.str





chain nodes :
1 2 3 4 11 12
ring nodes :
5 6 7 8 9 10

chain bonds :

1-2 2-3 3-4 4-5 8-11 11-12

ring bonds :

5-6 5-10 6-7 7-8 8-9 9-10

exact/norm bonds : 1-2 3-4 4-5 11-12

exact bonds : 2-3 8-11

normalized bonds :

5-6 5-10 6-7 7-8 8-9 9-10

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 12:CLASS

39 ANSWERS

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 07:21:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3363 TO ITERATE

59.5% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 63782 TO 70738

PROJECTED ANSWERS: 826 TO 1796

L2 39 SEA SSS SAM L1

=> d 1-39

L2 ANSWER 1 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 920259-55-8 REGISTRY

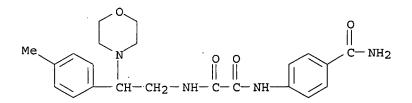
ED Entered STN: 09 Feb 2007

CN INDEX NAME NOT YET ASSIGNED

MF C22 H26 N4 O4

SR Chemical Library

Supplier: Aurora Fine Chemicals



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 2 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 920258-02-2 REGISTRY

ED Entered STN: 09 Feb 2007

CN INDEX NAME NOT YET ASSIGNED

MF C20 H24 N4 O4

SR Chemical Library

Supplier: Aurora Fine Chemicals

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 3 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 906151-24-4 REGISTRY

ED Entered STN: 10 Sep 2006

CN INDEX NAME NOT YET ASSIGNED

MF C22 H26 F N5 O3

SR Chemical Library

Supplier: Ambinter

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 4 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 885559-11-5 REGISTRY

ED Entered STN: 25 May 2006

CN Acetic acid, [[4-(aminocarbonyl)phenyl]amino]oxo-, [[3-[(2,4-dichlorophenyl)methoxy]phenyl]methylene]hydrazide (9CI) (CA INDEX NAME)

MF C23 H18 Cl2 N4 O4

SR Chemical Library

Supplier: Scientific Exchange, Inc.

LC STN Files: CHEMCATS

$$\begin{array}{c|c} C1 & & & & \\ \hline \\ C1 & & \\ \hline \\ C1 & & \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 5 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 885551-73-5 REGISTRY

ED Entered STN: 25 May 2006

CN Acetic acid, [[4-(aminocarbonyl)phenyl]amino]oxo-, [[3-bromo-4-[(4-chlorophenyl)methoxy]-5-ethoxyphenyl]methylene]hydrazide (9CI) (CA INDEX NAME)

MF C25 H22 Br Cl N4 O5

SR Chemical Library

Supplier: Scientific Exchange, Inc.

LC STN Files: CHEMCATS

C1

Br

$$CH = N - NH - C - C - NH$$

OEt

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 6 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 885546-88-3 REGISTRY

ED Entered STN: 25 May 2006

CN Benzoic acid, 2-methyl-, 2-[[[[[4-(aminocarbonyl)phenyl]amino]oxoacetyl]hy drazono]methyl]phenyl ester (9CI) (CA INDEX NAME)

MF C24 H20 N4 O5

SR Chemical Library

Supplier: Scientific Exchange, Inc.

LC STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 7 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 885534-75-8 REGISTRY

ED Entered STN: 25 May 2006

MF C24 H20 N4 O5

SR Chemical Library

Supplier: Scientific Exchange, Inc.

LC STN Files: CHEMCATS

L2ANSWER 8 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN885188-00-1 REGISTRY

ED Entered STN: 22 May 2006

Benzoic acid, 3-chloro-, 4-[[[[[4-(aminocarbonyl)phenyl]amino]oxoacetyl]hy CN drazono]methyl]phenyl ester (9CI) (CA INDEX NAME)

MF C23 H17 Cl N4 O5

Chemical Library SR

Supplier: Scientific Exchange, Inc.

LC STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ANSWER 9 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN L_2

885184-92-9 REGISTRY RN

ED

Entered STN: 22 May 2006
Acetic acid, [[4-(aminocarbonyl)phenyl]amino]oxo-, [[4-(diethylamino)-2-CN hydroxyphenyl]methylene]hydrazide (9CI) (CA INDEX NAME)

MF C20 H23 N5 O4

SR Chemical Library

Supplier: Scientific Exchange, Inc.

LC STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 10 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

885183-17-5 REGISTRY RN

ED

Entered STN: 22 May 2006
Acetic acid, [[4-(aminocarbonyl)phenyl]amino]oxo-, [[4-[(2-CN fluorophenyl)methoxy]-3-methoxyphenyl]methylene]hydrazide (9CI) (CA INDEX NAME)

MF C24 H21 F N4 O5

SR Chemical Library

Supplier: Scientific Exchange, Inc.

STN Files: LC CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 11 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

885167-04-4 REGISTRY RN

ED Entered STN: 22 May 2006

Acetic acid, [[4-(aminocarbonyl)phenyl]amino]oxo-, [1-[4-CN (phenylmethoxy)phenyl]ethylidene]hydrazide (9CI) (CA INDEX NAME)

MF C24 H22 N4 O4

Chemical Library SR

Supplier: Scientific Exchange, Inc.

LC STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ANSWER 12 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN L2

RN885162-48-1 REGISTRY

ED Entered STN: 22 May 2006

CN Acetic acid, [[4-(aminocarbonyl)phenyl]amino]oxo-, [[4-(2,4dinitrophenoxy)-3-methoxyphenyl]methylene]hydrazide (9CI) (CA INDEX NAME)

C23 H18 N6 O9 MF

SR Chemical Library

Supplier: Scientific Exchange, Inc.

STN Files: CHEMCATS LC

$$\begin{array}{c|c} O_2N & & & & & \\ \hline \\ NO_2 & & & \\ \end{array}$$

L2 ANSWER 13 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 885161-26-2 REGISTRY

ED Entered STN: 22 May 2006

CN Benzoic acid, 3-methyl-, 3-[[[[4-(aminocarbonyl)phenyl]amino]oxoacetyl]hy drazono]methyl]phenyl ester (9CI) (CA INDEX NAME)

MF C24 H20 N4 O5

SR Chemical Library

Supplier: Scientific Exchange, Inc.

LC STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 ANSWER 14 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 885154-04-1 REGISTRY
- ED Entered STN: 22 May 2006
- CN Acetic acid, [[4-(aminocarbonyl)phenyl]amino]oxo-, [[3-bromo-4-[(2-chloro-6-fluorophenyl)methoxy]-5-methoxyphenyl]methylene]hydrazide (9CI) (CA INDEX NAME)
- MF C24 H19 Br Cl F N4 O5
- SR Chemical Library

Supplier: Scientific Exchange, Inc.

LC STN Files: CHEMCATS

$$\begin{array}{c|c} C1 & \text{MeO} \\ \hline \\ CH_2 - O \\ \hline \\ F & Br \end{array}$$

L2 ANSWER 15 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 885139-62-8 REGISTRY

ED Entered STN: 22 May 2006

CN Butanoic acid, 3-[[[[4-(aminocarbonyl)phenyl]amino]oxoacetyl]hydrazono]-2-(hydroxyimino)-, ethyl ester (9CI) (CA INDEX NAME)

MF C15 H17 N5 O6

SR Chemical Library

Supplier: Scientific Exchange, Inc.

LC STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 16 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 850215-90-6 REGISTRY

ED Entered STN: 11 May 2005

CN Benzamide, 4-[[[(4-iodophenyl)amino]acetyl]amino]- (9CI) (CA INDEX NAME)

MF C15 H14 I N3 O2

SR Chemical Library

Supplier: Enamine

$$\begin{array}{c|c} & & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & \\ & & \\ &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 17 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 797784-55-5 REGISTRY

ED Entered STN: 15 Dec 2004

CN 5-Benzofuranacetamide, α -[[4-(aminoiminomethyl)phenyl]amino]-N[(dimethylamino)sulfonyl]-7-ethyl-3-methyl- (9CI) (CA INDEX NAME)

MF C22 H27 N5 O4 S

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 18 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 503130-93-6 REGISTRY

ED Entered STN: 16 Apr 2003

CN Carbamic acid, [(1S)-2-[[4-(aminocarbonyl)-2-iodophenyl]amino]-1-[(1,1-dimethylethoxy)methyl]-2-oxoethyl]-, 9H-fluoren-9-ylmethyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C29 H30 I N3 O5

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L2 ANSWER 19 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 481069-24-3 REGISTRY

ED Entered STN: 24 Jan 2003

CN Glycine, N-[[[4-[[[[4-(aminoiminomethyl)phenyl]amino]acetyl]amino]-2,5-dimethylphenyl](1-methylethyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

MF C23 H30 N6 O4

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 20 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 313491-49-5 REGISTRY

ED Entered STN: 11 Jan 2001

CN Benzeneacetamide, N-[4-(aminocarbonyl)phenyl]- α -[[3-(aminomethyl)benzoyl]amino]-, (α R)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C23 H22 N4 O3 . C2 H F3 O2

SR CA

LC STN Files: CA, CAPLUS

CM 1

CRN 313491-48-4 CMF C23 H22 N4 O3

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

- 3 REFERENCES IN FILE CA (1907 TO DATE)
- 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L2 ANSWER 21 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 284044-11-7 REGISTRY
- ED Entered STN: 08 Aug 2000
- CN Benzeneacetamide, α -[[4-(aminoiminomethyl)phenyl]amino]-3,5
 - dimethoxy-N-(propylsulfonyl)- (9CI) (CA INDEX NAME)
- MF C20 H26 N4 O5 S
- SR CA
- LC STN Files: CA, CAPLUS, USPATZ, USPATFULL

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L2 ANSWER 22 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 284043-72-7 . REGISTRY
- ED Entered STN: 08 Aug 2000
- CN Benzenecarboximidamide, 4-[[1-[3-methoxy-4-(phenylmethoxy)phenyl]-2-[[[3-(trifluoromethyl)phenyl]sulfonyl]amino]ethyl]amino]- (9CI) (CA INDEX NAME)
- MF C30 H29 F3 N4 O4 S
- SR CA
- LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

$$\begin{array}{c|c} NH \\ \parallel \\ C-NH_2 \\ \hline \\ Ph-CH_2-O \\ NH \\ \hline \\ CH-CH_2-NH-S \\ \hline \\ O \\ \hline \end{array}$$

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 23 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 284043-68-1 REGISTRY

ED Entered STN: 08 Aug 2000

CN Benzenecarboximidamide, 4-[[1-[3-methoxy-4-(phenylmethoxy)phenyl]-2-[(2-naphthalenylsulfonyl)amino]ethyl]amino]- (9CI) (CA INDEX NAME)

MF C33 H32 N4 O4 S

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 24 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 284043-62-5 REGISTRY

ED Entered STN: 08 Aug 2000

CN Benzoic acid, 3-[[[2-[[4-(aminoiminomethyl)phenyl]amino]-2-[3-methoxy-4-(phenylmethoxy)phenyl]ethyl]amino]sulfonyl]- (9CI) (CA INDEX NAME)

MF C30 H30 N4 O6 S

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L2 ANSWER 25 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 227024-17-1 REGISTRY
- ED Entered STN: 07 Jul 1999
- CN Benzeneacetamide, α-[[4-(aminoiminomethyl)phenyl]amino]-2,3,4trimethoxy-N-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)
- MF C25 H28 N4 O4 . x Cl H
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL
- CRN (709608-58-2)

$$\begin{array}{c|c} \text{NH} & \text{OMe} \\ \text{H}_2\text{N-C} & \text{MeO} & \text{OMe} \\ \\ \text{NH-CH} & \text{C-NH-CH}_2\text{-Ph} \\ \\ \text{O} & \\ \end{array}$$

●x HCl

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L2 ANSWER 26 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 227023-65-6 REGISTRY
- ED Entered STN: 07 Jul 1999
- CN Benzeneacetamide, 3-(acetylamino)- α -[[4- [(hydroxyamino)iminomethyl]phenyl]amino]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)
- MF C24 H25 N5 O3
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L2 ANSWER 27 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 227023-17-8 REGISTRY
- ED Entered STN: 07 Jul 1999
- CN Glycine, (2R)-N-[4-(aminoiminomethyl)phenyl]-2-[5-methoxy-4-(phenylmethoxy)-2-[(phenylsulfonyl)amino]phenyl]glycyl-2-phenyl-, (2S)-(9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C37 H35 N5 O7 S
- CI COM
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L2 ANSWER 28 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 227023-06-5 REGISTRY
- ED Entered STN: 07 Jul 1999
- CN Benzoic acid, 4-[4-[1-[[4-(aminoiminomethyl)phenyl]amino]-2-oxo-2-[(phenylmethyl)amino]ethyl]-2-methoxyphenoxy]- (9CI) (CA INDEX NAME)
- MF C30 H28 N4 O5
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

$$\begin{array}{c|c} O & NH \\ C-NH-CH_2-Ph & \parallel \\ C-NH_2 \\ \end{array}$$

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 29 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 227022-78-8 REGISTRY

ED Entered STN: 07 Jul 1999

CN Benzeneacetamide, α -[[4-(aminoiminomethyl)phenyl]amino]-2-(benzoylamino)-4,5-dimethoxy-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

MF C31 H31 N5 O4

CI COM

SR CA

$$\begin{array}{c|c} NH & O \\ \parallel & \parallel \\ Ph-C-NH & OMe \\ \hline NH-CH-CH-CH-CH & OMe \\ \hline Ph-CH_2-NH-C & \parallel \\ O & O \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 30 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 227022-63-1 REGISTRY

ED Entered STN: 07 Jul 1999

CN Benzeneacetamide, α -[[4-(aminoiminomethyl)phenyl]amino]-N-[(1R)-2-hydroxy-1-phenylethyl]-3-methoxy-4-(phenylmethoxy)-, (α R)-, monoacetate (salt) (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C31 H32 N4 O4 . C2 H4 O2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 227022-62-0 CMF C31 H32 N4 O4

Absolute stereochemistry.

CM 2

CRN 64-19-7 CMF C2 H4 02

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 31 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 227022-41-5 REGISTRY

ED Entered STN: 07 Jul 1999

CN Butanoic acid, 4-amino-2-[[[[4-(aminoiminomethyl)phenyl]amino][3-methoxy-4-(phenylmethoxy)phenyl]acetyl]amino]-, (2S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C27 H31 N5 O5

CI COM

SR CA

Absolute stereochemistry.

$$H_2N$$
 S
 N
 CO_2H
 NH_2
 NH_2
 NH_2
 NH_2
 NH_2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 32 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 227022-29-9 REGISTRY

ED Entered STN: 07 Jul 1999

CN L-Alanine, (2S)-N-[4-(aminoiminomethyl)phenyl]-2-[3-methoxy-4-

(phenylmethoxy)phenyl]glycyl-3-[[(1,1-dimethylethoxy)carbonyl]amino]-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C31 H37 N5 O7

CI COM SR CA

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 33 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 227021-99-0 REGISTRY

ED Entered STN: 07 Jul 1999

CN L-Tyrosine, (2R)-N-[4-(aminoiminomethyl)phenyl]-2-[3-methoxy-4-(phenylmethoxy)phenyl]glycyl- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C32 H32 N4 O6

CI COM

SR CA

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 34 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 227021-88-7 REGISTRY

ED Entered STN: 07 Jul 1999

CN Carbamic acid, [[4-[[1-(3,4-dimethoxyphenyl)-2-oxo-2-[(phenylmethyl)amino]ethyl]amino]phenyl]iminomethyl]-, methyl ester (9CI) (CA INDEX NAME)

MF C26 H28 N4 O5

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 35 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 227021-10-5 REGISTRY

ED Entered STN: 07 Jul 1999

CN Benzeneacetamide, α -[[4-(aminoiminomethyl)phenyl]amino]-3-methoxy-N-phenyl-4-(phenylmethoxy)-, acetate (9CI) (CA INDEX NAME)

MF C29 H28 N4 O3 . x C2 H4 O2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 227021-09-2 CMF C29 H28 N4 O3

$$\begin{array}{c|c} & \text{NH} & \text{OMe} \\ H_2N-C & R & \text{O-CH}_2-Ph \\ \hline & NH-CH & \end{array}$$

CM 2

CRN 64-19-7 CMF C2 H4 O2

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 36 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 227020-88-4 REGISTRY

ED Entered STN: 07 Jul 1999

CN Benzeneacetamide, α -[[4-(aminoiminomethyl)phenyl]amino]-3-methoxy-4-(2-phenylethoxy)-N-(phenylmethyl)-, acetate (9CI) (CA INDEX NAME)

MF C31 H32 N4 O3 . x C2 H4 O2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 227020-87-3 CMF C31.H32 N4 O3

$$\begin{array}{c|c} \text{NH} & \text{O} \\ \parallel & \parallel \\ \text{H}_2\text{N-C} & \parallel \\ \text{C-NH-CH}_2\text{-Ph} \\ \hline \\ \text{NH-CH} & \text{O-CH}_2\text{-CH}_2\text{-Ph} \\ \\ \text{OMe} \end{array}$$

CM 2

CRN 64-19-7 CMF C2 H4 O2

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L2 ANSWER 37 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 227020-71-5 REGISTRY
- ED Entered STN: 07 Jul 1999
- CN Benzeneacetamide, α -[[4-(aminoiminomethyl)phenyl]amino]-3-methoxy-4-[(3-methoxyphenyl)methoxy]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)
- MF C31 H32 N4 O4
- CI COM
- SR CA

MeO
$$CH_2 - OH_2$$
 $CH_2 - OH_2$ $CH_2 - OH_2$

L2 ANSWER 38 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN

RN 227020-58-8 REGISTRY

ED Entered STN: 07 Jul 1999

CN Benzeneacetamide, α -[[4-(aminoiminomethyl)phenyl]amino]-3-methoxy-4-(phenylmethoxy)-N-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

MF C30 H30 N4 O3 . \times C2 H F3 O2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 227020-57-7 CMF C30 H30 N4 O3

$$\begin{array}{c|c} NH & O \\ \parallel & \parallel \\ H_2N-C & \parallel \\ NH-CH & O-CH_2-Ph \\ \hline OMe & O-CH_2-Ph \\ \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L2 ANSWER 39 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 90291-90-0 REGISTRY
- ED Entered STN: 16 Nov 1984
- CN Benzenepropanamide, N-[4-(aminoiminomethyl)phenyl]- α -[[(4-methylphenyl)sulfonyl]amino]-, monohydriodide (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

Benzenepropanamide, N-[4-(aminoiminomethyl)phenyl]- α -[[(4methylphenyl) sulfonyl] amino] -, monohydriodide, (\pm) -

MF C23 H24 N4 O3 S . H I

STN Files: BEILSTEIN*, CA, CAPLUS LC

(*File contains numerically searchable property data)

(92953-67-8) CRN

● HI

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> s l1 esa

COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID The query entered contains both search terms created by structure-building or screen commands and text search terms. L#s created via the STRUCTURE or SCREEN commands must be searched in the structures files separately from text terms or profiles. The L# answer sets from structure searches can be used in crossover searches and can be combined with text terms.

=> s l1 exa

SAMPLE SEARCH INITIATED 07:23:04 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -0 TO ITERATE

100.0% PROCESSED

0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

0 TO 0

0 TO

PROJECTED ANSWERS:

L3

O SEA EXA SAM L1

Uploading C:\Documents and Settings\mgraffeo\My Documents\Critical Data\10814058\cmp 3.str

chain nodes :
1 2 3 4 11
ring nodes :
5 6 7 8 9 10
chain bonds :
1-2 2-3 3-4 4-5 8-11
ring bonds :
5-6 5-10 6-7 7-8 8-9 9-10
exact/norm bonds :
1-2 3-4 4-5

exact bonds : 2-3 8-11 normalized bonds : 5-6 5-10 6-7 7-8 8-9 9-10

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS

L4 STRUCTURE UPLOADED

=> s 14 exa SAMPLE SEARCH INITIATED 07:24:03 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 5 TO 234

PROJECTED ANSWERS: 0 TO 0

L5 0 SEA EXA SAM L4

=> s 14 full FULL SEARCH INITIATED 07:24:16 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 126827 TO ITERATE

100.0% PROCESSED 126827 ITERATIONS 25959 ANSWERS

SEARCH TIME: 00.00.02

L6 25959 SEA SSS FUL L4

=> s 16 esa
MISSING OPERATOR

=> s 16 exa,

SAMPLE SEARCH INITIATED 07:24:32 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.05

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 5 TO 234

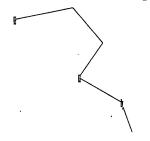
PROJECTED ANSWERS:

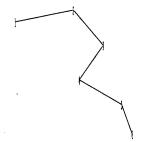
0 TO

L7 0 SEA EXA SAM L4

=> Uploading C:\Documents and Settings\mgraffeo\My Documents\Critical

Data\10814058\cmp 4.str





50 ANSWERS

chain nodes:
1 2 3 4 5 6

chain bonds :

1-2 2-3 3-4 4-5 5-6

exact/norm bonds : 1-2 3-4 4-5 5-6

exact bonds :

2-3

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS

L8 STRUCTURE UPLOADED

=> s 18

SAMPLE SEARCH INITIATED 07:27:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 149556 TO ITERATE

1.3% PROCESSED 2000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 2968301 TO 3013939

PROJECTED ANSWERS: 112074 TO 121232

L9 50 SEA SSS SAM L8

=> s 18 exa
STRUCTURES CONTAINING VARIABLE NODES NOT VALID IN EXACT OR FAMILY SEARCH
You have requested a full structure (EXA or FAM) search on a
structure containing one of the special variable-atom symbols
A, M, Q, or X, or a variable group G. Only bond variability

is allowed in structures for EXA or FAM searches. Variable nodes are never permitted.

=> s 19

SAMPLE SEARCH INITIATED 07:27:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 149556 TO ITERATE

1.3% PROCESSED 2000 ITERATIONS

TERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS:

2968301 TO 3013939

PROJECTED ANSWERS:

112074 TO 121232

L10

50 SEA SSS SAM L8

=> d 1-20

L10 ANSWER 1 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN

RN 920323-68-8 REGISTRY

ED Entered STN: 09 Feb 2007

CN L-Argininamide, L-norleucyl-L-cysteinyl-L-histidyl-D-phenylalanyl-L-arginyl-L-tryptophyl-4-aminobutanoyl-L-cysteinyl-β-alanyl-β-alanyl-L-tyrosylglycyl-L-arginyl-

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C124 H205 N57 O24 S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

PAGE 1-C

$$H_{2N}$$
 H_{2N}
 H

PAGE 2-B

PAGE 3-B

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 2 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN

RN 920254-75-7 REGISTRY

ED Entered STN: 09 Feb 2007

CN Ethanediamide, N1-(4-methyl-2-thiazolyl)-N2-(2-thienylmethyl)- (CA INDEX NAME)

MF C11 H11 N3 O2 S2

SR Chemical Library

Supplier: Aurora Fine Chemicals

Me NH-C-C-NH-CH₂
$$\stackrel{\circ}{\underset{S}{\longrightarrow}}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 ANSWER 3 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN

RN 917106-88-8 REGISTRY

ED Entered STN: 10 Jan 2007

CN Benzamide, 2,5-dichloro-N-[2-[[(3-endo)-8-[(4-chlorophenyl)methyl]-8-

azabicyclo[3.2.1]oct-3-yl]amino]-2-oxoethyl]- (CA INDEX NAME)

FS STEREOSEARCH

MF C23 H24 Cl3 N3 O2

SR CA

LC STN Files: CA, CAPLUS

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 4 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN

RN 903199-11-1 REGISTRY

ED Entered STN: 22 Aug 2006

CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 4,7-dihydro-5,5-dimethyl-2-[[2-[[[4-(1-methylethoxy)phenyl]methyl]amino]-2-oxoacetyl]amino]- (CA INDEX NAME)

MF C22 H26 N2 O6 S

SR Chemical Library

Supplier: Interbioscreen Ltd.

LC STN Files: CHEMCATS

$$\begin{array}{c|c} & \circ & \circ \\ & \circ & \circ \\ & \text{Me} & \text{NH-C-C-NH-CH}_2 \end{array} \\ & \text{OPr-i} \\ & \text{Me} & \text{CO}_2\text{H} \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 ANSWER 5 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN

RN 889936-52-1 REGISTRY

ED Entered STN: 29 Jun 2006

CN Vancomycin, N3''-[[3-[[(3,4-dichlorophenyl)acetyl]amino]-4-(4-morpholinylamino)phenyl]methyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C85 H94 Cl4 N12 O26

CI COM

SR CA

Absolute stereochemistry.

ОН

PAGE 2-A

PAGE 2-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 ANSWER 6 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN

RN 885544-08-1 REGISTRY

ED Entered STN: 25 May 2006

CN INDEX NAME NOT YET ASSIGNED

MF C28 H26 Br N3 O7 S

SR Chemical Library

Supplier: Scientific Exchange, Inc.

LC STN Files: CHEMCATS

L10 ANSWER 7 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN

RN 880879-26-5 REGISTRY

ED Entered STN: 18 Apr 2006

CN L-Tyrosine, L-seryl-L-α-aspartyl-L-seryl-L-lysyl-L-isoleucylglycyl-L-asparaginylglycyl-L-cysteinyl-L-phenylalanylglycyl-L-phenylalanyl-L-prolyl-L-leucyl-L-α-aspartyl-L-arginyl-L-isoleucylglycyl-L-seryl-L-valyl-L-serylglycyl-L-leucylglycyl-L-cysteinyl-L-asparaginyl-L-seryl-L-phenylalanyl-L-arginyl-, cyclic (9→25)-disulfide (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 112: PN: WO2006005140 SEQID: 126 claimed protein

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C137 H207 N39 O43 S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

PAGE 1-B



PAGE 2-A

HO
$$(CH_2)_3$$
 O NH HO $(CH_2)_3$ O $(CH_2$

но

PAGE 2-C

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 8 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN

RN 872181-10-7 REGISTRY

ED Entered STN: 19 Jan 2006

CN L-Cysteine, N6-[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'[9H]xanthen]-5-yl)amino]thioxomethyl]-L-lysylglycyl-L-cysteinyl-Lasparaginylglycyl-L-arginyl-, cyclic (3→7)-disulfide (9CI) (CA
INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C47 H57 N13 O14 S3 ·

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L10 ANSWER 9 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 861888-37-1 REGISTRY
- ED Entered STN: 26 Aug 2005
- CN L-Glutamamide, N-acetyl-L-tyrosyl-L-glutaminyl-3-mercapto-L-valyl-L-typtophyl-L-arginyl-L-tyrosyl-L-cysteinyl-, cyclic (3→7)-disulfide (9CI) (CA INDEX NAME)
- FS PROTEIN SEQUENCE; STEREOSEARCH
- MF C55 H73 N15 O13 S2
- SR CA
- LC STN Files: CA, CAPLUS, CASREACT

PAGE 1-B

PAGE 2-A

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 10 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN

RN 854914-73-1 REGISTRY

ED Entered STN: 13 Jul 2005

CN Piperidinium, 1-[(3-chlorophenyl)methyl]-3-[[(2S)-3-(4-hydroxyphenyl)-2-[[[[4-(2-methyl-1-oxopropoxy)phenyl]amino]carbonyl]amino]-1oxopropyl]amino]-1-methyl-, (3S)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C33 H40 Cl N4 O5 . C2 F3 O2

SR CA

LC STN Files: CA, CAPLUS

CM 1

CRN 854914-72-0 CMF C33 H40 Cl N4 O5

Absolute stereochemistry.

CM 2

CRN 14477-72-6 CMF C2 F3 O2

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L10 ANSWER 11 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 850412-33-8 REGISTRY
- ED Entered STN: 13 May 2005
- CN Carbamic acid, [2-[[[2-oxo-2-[[(3R)-1-(phenylmethyl)-3-pyrrolidinyl]amino]ethyl]amino]carbonyl]-4-(trifluoromethoxy)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C26 H31 F3 N4 O5
- SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L10 ANSWER 12 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 849242-48-4 REGISTRY
- ED Entered STN: 26 Apr 2005
- CN 1,4-Dithia-7,10-diazacyclotridecane-6-carboxamide, 12-[[(2S)-2-amino-3-(4-hydroxyphenyl)-1-oxopropyl]amino]-9-(1H-indol-3-ylmethyl)-8,11-dioxo-, (6S,9S,12S)- (9CI) (CA INDEX NAME)
- FS PROTEIN SEQUENCE; STEREOSEARCH
- MF C28 H34 N6 O5 S2
- SR CA
- LC STN Files: CA, CAPLUS, CASREACT

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L10 ANSWER 13 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 845898-97-7 REGISTRY
- ED Entered STN: 18 Mar 2005

CN Benzeneacetamide, 3,5-difluoro-N-[1-[[[5-[3-[(2-hydroxyethyl)amino]-1,1-dimethylpropyl]-1,3,4-thiadiazol-2-yl]amino]carbonyl]butyl]- (9CI) (CA INDEX NAME)

MF C22 H31 F2 N5 O3 S

CI COM

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 14 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN

RN 843643-68-5 REGISTRY

ED Entered STN: 07 Mar 2005

CN Benzeneacetamide, 3,5-difluoro-N-[1-[[[5-[1-(4-morpholinyl)ethyl]-2-pyridinyl]amino]carbonyl]butyl]- (9CI) (CA INDEX NAME)

MF C24 H30 F2 N4 O3

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 15 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN

RN 802004-89-3 REGISTRY

ED Entered STN: 22 Dec 2004

CN 2-Thiophenecarboxylic acid, 4-(2-guanidinoacetamido)-5-methyl- (8CI) (CA INDEX NAME)

MF C9 H12 N4 O3 S

CI COM

SR CA

L10 ANSWER 16 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN

RN 785759-57-1 REGISTRY

ED Entered STN: 22 Nov 2004

CN 2-Pyrrolidinecarboxamide, 4-[[(2S)-2-amino-3-hydroxy-1-oxopropyl]amino]-1-[(2S)-2-amino-1-oxo-4-phenylbutyl]-N-(2,3-dihydro-1H-inden-5-yl)-, (2S,4R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C27 H35 N5 O4

CI COM

SR CA

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 ANSWER 17 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN

RN 770675-09-7 REGISTRY

ED Entered STN: 27 Oct 2004

CN 6H-Pyrazolo[4,5,1-de]acridin-6-one, 2-[[[2-(dimethylamino)ethyl]amino]meth yl]-7-hydroxy-5-[[2-[(2-hydroxyethyl)amino]ethyl]amino]- (9CI) (CA INDEX NAME)

MF C23 H30 N6 O3

CI COM

SR CA

L10 ANSWER 18 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN

RN 762291-00-9 REGISTRY

ED Entered STN: 14 Oct 2004

CN Benzeneacetamide, 3,5-difluoro-N-[(1S)-1-methyl-2-oxo-2-[[(3S)-2,3,6,7-tetrahydro-1-methyl-2-oxo-5-phenyl-1H-azepin-3-yl]amino]ethyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C24 H25 F2 N3 O3

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 19 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN

RN 757138-32-2 REGISTRY

ED Entered STN: 05 Oct 2004

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[[1,4-dihydro-2[(4-nitrophenyl)amino]-4-oxo-5-pyrimidinyl]amino]carbonyl]amino](4hydroxyphenyl)acetyl]amino]-3,3-dimethyl-7-oxo-, [2S[2α,5α,6β(S*)]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C27 H26 N8 O9 S

CI COM

SR CA

Absolute stereochemistry.

L10 ANSWER 20 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN

RN 748734-75-0 REGISTRY

ED Entered STN: 20 Sep 2004

CN 2,4(1H,3H)-Pyrimidinedione, 6-[[2-[[3-(4-chloro-3,5-dimethylphenoxy)-2-hydroxypropyl]amino]ethyl]amino]-1,3-dimethyl- (9CI) (CA INDEX NAME)

MF C19 H27 Cl N4 O4

CI COM

SR CA

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST

303.35 303.77

STN INTERNATIONAL LOGOFF AT 07:43:04 ON 07 MAY 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptamxg1614

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

```
Welcome to STN International
NEWS
                 Web Page URLs for STN Seminar Schedule - N. America
NEWS
         JAN 08
                 CHEMLIST enhanced with New Zealand Inventory of Chemicals
                 CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS
     3. JAN 16
                 IPC version 2007.01 thesaurus available on STN
NEWS 4
         JAN 16
NEWS 5
         JAN 16
                 WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
                 CA/CAplus updated with revised CAS roles
NEWS 6
         JAN 22
         JAN 22
                 CA/CAplus enhanced with patent applications from India
NEWS
     7
NEWS 8
         JAN 29
                 PHAR reloaded with new search and display fields
NEWS 9
                 CAS Registry Number crossover limit increased to 300,000 in
         JAN 29
                 multiple databases
                 PATDPASPC enhanced with Drug Approval numbers
NEWS 10
         FEB 15
NEWS 11
        FEB 15
                 RUSSIAPAT enhanced with pre-1994 records
NEWS 12
        FEB 23
                 KOREAPAT enhanced with IPC 8 features and functionality
                 MEDLINE reloaded with enhancements
NEWS 13
        FEB 26
                 EMBASE enhanced with Clinical Trial Number field
NEWS 14
        FEB 26
                 TOXCENTER enhanced with reloaded MEDLINE
NEWS 15
        FEB 26
NEWS 16
         FEB 26
                 IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 17
         FEB 26
                 CAS Registry Number crossover limit increased from 10,000
                 to 300,000 in multiple databases
                 WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 18
        MAR 15
NEWS 19
        MAR 16
                 CASREACT coverage extended
NEWS 20
        MAR 20
                 MARPAT now updated daily
NEWS 21 MAR 22
                LWPI reloaded
NEWS 22 MAR 30
                RDISCLOSURE reloaded with enhancements
NEWS 23 APR 02
                JICST-EPLUS removed from database clusters and STN
NEWS 24 APR 30 GENBANK reloaded and enhanced with Genome Project ID field
NEWS 25 APR 30
                CHEMCATS enhanced with 1.2 million new records
NEWS 26 APR 30
                 CA/CAplus enhanced with 1870-1889 U.S. patent records
                 INPADOC replaced by INPADOCDB on STN
NEWS 27
        APR 30
NEWS 28 MAY 01
                New CAS web site launched
NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
NEWS HOURS
              STN Operating Hours Plus Help Desk Availability
NEWS LOGIN
              Welcome Banner and News Items
              For general information regarding STN implementation of IPC 8
NEWS IPC8
```

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY 0.63 SESSION 0.63

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 09:43:52 ON 07 MAY 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 MAY 2007 HIGHEST RN 934336-20-6 DICTIONARY FILE UPDATES: 6 MAY 2007 HIGHEST RN 934336-20-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

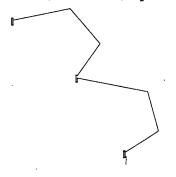
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

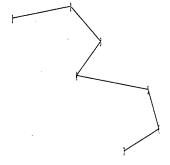
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

Uploading C:\Documents and Settings\mgraffeo\My Documents\Critical Data\10814058\cmp 5.str





chain nodes :

1 2 3 4 5 6 7

chain bonds :

1-2 2-3 3-4 4-5 5-6 6-7

exact/norm bonds : 1-2 3-4 4-5 6-7

exact bonds : 2-3 5-6

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS

L1 STRUCTURE UPLOADED

=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

1.08

0.45

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 09:44:04 ON 07 MAY 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 MAY 2007 HIGHEST RN 934336-20-6 DICTIONARY FILE UPDATES: 6 MAY 2007 HIGHEST RN 934336-20-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> s l1

SAMPLE SEARCH INITIATED 09:44:07 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 94634 TO ITERATE

2.1% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

50 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 1874416 TO 1910944 PROJECTED ANSWERS: 746386 TO 769650

L2 50 SEA SSS SAM L1

=> s l1 exa

SAMPLE SEARCH INITIATED 09:44:15 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 13 TO ITERATE

100.0% PROCESSED 13 ITERATIONS SEARCH TIME: 00.00.01

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

```
BATCH
        **COMPLETE**
```

PROJECTED ITERATIONS:

44 TO 476 1 TO

PROJECTED ANSWERS:

1 SEA EXA SAM L1

=> d

L3

ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN L3

RN 756798-35-3 REGISTRY

Entered STN: 05 Oct 2004 ED

CN 1,2-Ethanedi(amine-15N), N-[2-(amino-15N)ethyl]- (9CI) (CA INDEX NAME)

MF C4 H13 N3

CI COM

SR CA

 $15NH_2 - CH_2 - CH_2 - 15NH - CH_2 - CH_2 - 15NH_2$

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

2.40 3.48

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 09:44:40 ON 07 MAY 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 7 May 2007 VOL 146 ISS 20 FILE LAST UPDATED: 6 May 2007 (20070506/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> s 13

0 L3 L4

=> s 756798-35-3/rn

0 756798-35-3

0 756798-35-3D L50 756798-35-3/RN

(756798-35-3 (NOTL) 756798-35-3D)

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

4.49

7.97

STN INTERNATIONAL LOGOFF AT 09:45:33 ON 07 MAY 2007